TECHNICAL REPORT

Office of Naval Research Contract No. N00014-86-K0029

A FURTHER NOTE ON GENERALIZED HYPEREXPONENTIAL DISTRIBUTIONS

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Carl M. Harris
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Report No. GMU/22474/112
November 15, 1989

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Copy No. 20

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) A Further Note on Generalized Hyperexponential Distributions		5. TYPE OF REPORT & PERIOD COVERED Technical Report
		6. PERFORMING ORG. REPORT NUMBER GMU / 22474 / 112
7. AUTHOR(s) Carl M. Harris William G. Marchal Robert F. Botta		8. CONTRACT OR GRANT NUMBER(s) N00014-86-K0029
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Operations Research and Applied Statistics - George Mason University Fairfax, VA 22030		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Task H-B Project 4118150
11. CONTROLLING OFFICE NAME AND ADDRESS		12. REPORT DATE November 15, 1989
		13. NUMBER OF PAGES 19
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report)		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) applied probability computational analysis computatonal probability distributions Laplace transforms	Markov chains numerical methods probability queues stochastic models	
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) (see following)		

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

S/N 0102-LF-014-6601

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

A Further Note on Generalized Hyperexponential Distributions

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ABSTRACT

In this note, we update some earlier results on the relationship of generalized hyperexponential (GH) distributions to other types of CDFs in the Coxian family, particularly the phase types. Most specifically, we utilize properties of these Coxian-type distributions to offer some new approaches to determining when a given rational transform can be associated with a GH distribution.

1 INTRODUCTION

Many authors have used distribution functions related to the exponential-staging formulation introduced by Erlang (see Brockmeyer et al., 1948), with primary modifications over the years by Jensen (1954) and Cox (1955). Much of the current popularity of such distributions is due to the work of Neuts and colleagues on the so-called phase-type family (see, e.g., Neuts, 1975a,b and 1981), exploiting relationships to the theory of Markov chains and putting the theory to effective computational use in a large variety of stochastic models.

For purposes of clarity, we note the following relationships between these classes of cumulative distribution functions (CDFs). Essentially, all of this stems from Erlang's early idea of modeling a duration or lifetime as a sum of independent and identical exponential stages. Much later, Jensen (1954) generalized Erlang's device to allow the stages to have non-identical CDFs, and indeed recognized the natural connection between Erlang's method of stages and absorption-time distributions of finite Markov chains. (KR)

An important milestone came shortly thereafter in work by Cox (1955), who further generalized to cover all distributions with rational Laplace transforms, by involving a more complicated stage-to-stage movement, possibly using negative and/or imaginary branching "probabilities" and scale parameters (with negative real parts). While such stages may not necessarily have a physical reality, the differential equations can be formed in the usual way and the resulting CDF can well be legitmate. This class is commonly abbreviated as R_n and it contains the class of all phase-type distributions, which, in turn, contains all of Jensen's generalized Erlangs.

Some recent work by the current authors, together with a number of different coauthors, has focused on the generalized mixed exponential form (called GH) of Coxian CDF (see Botta & Harris, 1986; Botta, Harris & Marchal, 1987; and Harris & Sykes, 1987). These are linear, but not necessarily convex combinations of negative exponential CDFs:

$$F(t) = 1 - \sum_{i=1}^{n} p_i e^{-\lambda_i t}, \tag{1}$$

$$\lambda_i > 0; \ \sum_{i=1}^{n} p_i = 1, \ -\infty < p_i < \infty.$$

and

$$\lambda_1 < \lambda_2 < \ldots < \lambda_n \ (with\, no\, loss\, in\, generality).$$

Botta and Harris (1986) showed, critically, that the GH class is dense in the set of all CDFs relative to an appropriate metric. Denseness is also a property of both the PH and Coxian classes.

Shanthikumar (1985) worked with two classes of functions, which he called generalized and bilateral phase types. The CDF of the generalized phase type (GPH) is created from infinite mixing on the number of convolutions. The bilateral phase type is defined over the entire real line in an analogous fashion using Erlang mixing. It follows that a GPH distribution is an ordinary PH whenever the mixing distribution has finite support or has an infinite phase-type representation. Ott (1987) renamed the GPH distributions as almost phase types (APH) and employed the results in modeling the G/G/1 queue.

An additional class of CDFs was offered by Sumita and Masuda (1987), going back to the Cox idea of building on the nature of the transform and then working backward to the form of the CDF. This is the class (called Ω^+) of probability distribution functions which have Laplace-Stieltjes transforms with only real negative zeros and poles. Clearly, all such transforms are rational and thus $\Omega^+ \in R_n$. Since all the poles are real and negative, it appears at first glance that such CDFs should also be generalized hyperexponentials whenever these poles are distinct. However, such is not the case.

For a counterexample, consider the transform

$$f^*(s) = \frac{6}{13}\frac{2s^2 + 10s + 13}{(s+1)(s+2)(s+3)},$$

which is easily inverted to be the GH density

$$f(t) = \frac{15}{13}(e^{-t}) - \frac{3}{13}(2e^{-2t}) + \frac{1}{13}(3e^{-3t}). \tag{2}$$

However, we see that f(t) is not in Ω^+ since the roots of the numerator of $f^*(s)$ are complex. Clearly, this is not a pathological counterexample, for there are many examples of GH densities which have similar transform constructs. Another illustration is Example 2.2.2 (page 124) of Botta, Harris and Marchal (1987), namely,

$$f(t) = 4(e^{-t}) - 6(2e^{-2t}) + 3(3e^{-3t}).$$

The numerator of its transform is the polynomial $(s^2 - s + 6)$, which also has complex roots.

O'Cinneidem (1989) has recently introduced the properties of phase-type simplicity and majorization as aids in understanding the class of phase-type distributions. These results become useful when trying to determine when a given phase-type distribution may have multiple, distinct representations of the same Markov chain. But this search to learn how, where and why phase-type distributions have non-unique representations is, of course, predicated on their special nature, for non-uniqueness is not a property of all Coxian subclasses. For example, it is easy to show by basic algebraic properties that each distribution in the GH class is truly unique.

Note that O'Cinneidem's use of the term Coxian is inconsistent with the model proposed by Cox (1955), as discussed above, by a restriction that the mixing parameters be true probabilities on (0,1) and that the means of the exponential stages to be positive, *real* values. Therefore, it clearly follows that the Coxians so defined produce a class equivalent to that of the mixed generalized Erlangs (MGEs). (We prefer the term MGE over MCE for mixed convolutions of exponentials, because the latter would appear to connote mixtures of self-convolutions.)

The object of the present paper, then, is to clarify some issues relating the important subclasses of the Coxian set and then to try to resolve the major pending issue in the use of generalized hyperexponential distributions, namely, the establishment of effective procedures for testing whether any given linear combination of negative exponential functions is a legitimate probability distribution.

2 THEORETICAL SUFFICIENT CONDITIONS FOR GH

The major focus of this paper is the ability to use the results contained in all of the foregoing pieces on Coxian-type distributions to get a better picture of the basic makeup of the GH class. As noted, we are especially interested

in learning how to verify that a given generalized mixed exponential form is indeed a legitimate GH CDF. In this section, we shall employ the algebraic and probabilistic properties of the R_n class and its subsets to derive some tools for checking whether a particular generalized exponential mixture is indeed a *proper distribution* function. In the following section, we give strictly computational and graphical approaches to sufficiency.

Some key clues to this are found in Sumita and Masuda (1987). The class Ω^+ they have defined contains densities admitting Laplace transforms

$$f^*(s) = \frac{\prod_{i=1}^{m}(1 + s/\eta_i)}{\prod_{j=1}^{n}(1 + s/\theta_j)}, \tag{3}$$

$$(0 \leq m < n < \infty; \eta_i \neq \theta_j, \eta_i, \theta_j > 0 \; for \; all \; i, j).$$

(We assume that the numerator is 1 for $m = 0$.) Clearly, all such transforms are rational and thus $\Omega \subset R_n$; but, as we have already shown, Ω^+ is not a subset of the GH class.

Some of the major results of Sumita and Masuda (1987) have direct application to the more general class R_n and to the generalized hyperexponential distributions. A prime example of these is their Theorem 1.2, which provides a simple sufficient condition for $f \in GH$ when f is also in Ω^+. We have been able to extend their argument to derive a sufficient condition for $f \in GH$ independent of whether it is in Ω^+.

The condition offered by Sumita and Masuda requires that there exists an indexing of the $\{\theta_j\}$ and $\{\eta_i\}$ (assuming that $\eta_1 < \eta_2 < \ldots < \eta_m$ and $\theta_1 < \theta_2 < \ldots < \theta_n$) in which $\theta_i < \eta_i$, $1 \leq i \leq m$. A quick proof may be constructed by writing the transform as the product of n quotients of linear rational functions. The inverse transform of each of m factors is of the form

$$F_i(t) = \frac{\theta_i}{\eta_i} + \left(1 - \frac{\theta_i}{\eta_i}\right)\left(1 - e^{-\theta_i t}\right).$$

The requirement that $\theta_i < \eta_i$ thus yields a mixture of an atom at the origin and a negative exponential term. Each of the remaining $n - m$ terms corresponds to an ordinary negative exponential. Since each of the total of n terms corresponds to a legitimate probability distribution, the convolution will yield a true distribution (without an atom since there is at least one purely exponential term in the convolution).

Now suppose that the numerator polynomial of (3) can have complex roots occurring in conjugate pairs. Without too much difficulty, using an argument similar to the above, we can verify the following lemma, offered here without proof. (Some of the prior material and the following lemma are improved versions of material found in a prior report prepared under this grant by Harris and Botta, 1988.)

Lemma 1: *Suppose that a rational transform can be written for $0 < m < n$ as*

$$f^*(s) = \frac{\prod_{i=1}^{m}(1 + s/\eta_i)}{\prod_{j=1}^{m}(1 + s/\theta_j)},$$

where the $\{\theta_j\}$ are real, positive and arranged in ascending order, and the $\{\eta_i\}$ are either real and positive or occur in complex conjugate pairs with positive real parts. Suppose (without loss of generality) that

$$Re(\eta_1) \leq Re(\eta_2) \leq \ldots \leq Re(\eta_m)$$

(where equality holds only in the case of complex conjugates) and that, for $i = 1, 2, \ldots, m$, $\theta_i < \eta_i$ when η_i is real and $(\theta_i + \theta_{i+1})/2 \leq Re(\eta_i)$ when (η_i, η_{i+1}) are a complex conjugate pair. Then the inverse transform of $f^*(s)$ is a probability distribution.

To illustrate, consider the following examples. First, let

$$f^*(s) = \frac{(1 + \frac{s}{2+2i})(1 + \frac{s}{2-2i})}{(1 + s)(1 + s/2)(1 + s/3)}.$$

This transform does indeed come from a CDF since

$$\frac{\theta_1 + \theta_2}{2} = \frac{3}{2} < Re(\eta_1) = 2.$$

Alternatively, we can verify the result by computing the inverses of

$$f_1^*(s) = \frac{(1 + \frac{s}{2+2i})(1 + \frac{s}{2-2i})}{(1 + s)(1 + s/2)}$$

and

$$f_1^*(s) = 1/(1 + s/3)$$

and then convolving. We find that

$$F_1(t) = \frac{1}{4} + \frac{5}{4}(1 - e^{-t}) - \frac{1}{2}(1 - e^{-2t})$$

$$= \frac{1}{4} + \frac{3}{4}\left[\frac{5}{3}(1 - e^{-t}) - \frac{2}{3}(1 - e^{-2t})\right]$$

and

$$F_2(t) = 1 - e^{-3t}.$$

The absolutely continuous part of $F_1(t)$ is a legitimate distribution since $5e^{-t} > 4e^{-2t}$ for all t. Since $F_2(t)$ is a standard exponential CDF, it follows that $F(t)$ is a CDF.

As a second illustration, consider $F(t) = 1 - e^{-t} + e^{-2t} - e^{-3t}$, with

$$f^*(s) = \frac{(1 + \frac{s}{(3+\sqrt{3}i)/2})(1 + \frac{s}{(3-\sqrt{3}i)/2})}{(1 + s)(2 + s)(3 + s)}.$$

By taking

$$\eta_1 = \frac{3 + \sqrt{3}i}{2}, \ \eta_2 = \overline{\eta_1}, \ \theta_1 = 1, \ \theta_2 = 2,$$

we have

$$\frac{\theta_1 + \theta_2}{2} = \frac{3}{2} < Re(\eta_1) = 3,$$

so that the condition of the lemma is satisfied and this is also a CDF.

As a test for whether or not a linear combination of exponentials is a probability density, the above procedure is somewhat awkward (though powerful) since the transform must first be established. A more direct, sufficient condition was established by Bartholomew (1969) (following the work of Zemanian, 1959, 1961), based on the function's behavior at the origin. For the three-term model,

$$f(t) = a_1 e^{-\lambda_1 t} + a_2 e^{-\lambda_2 t} + a_3 e^{-\lambda_3 t} \quad (\lambda_1 < \lambda_2 < \lambda_3),$$

the conditions are

$$\begin{cases} 0 \leq f(0) \\ 0 \leq \lambda_3 f(0) + f'(0) \\ 0 \leq \lambda_3\lambda_2 f(0) + (\lambda_3 + \lambda_2) f'(0) + f''(0) \end{cases}.$$

To illustrate, let us consider the second of the two (potential) densities of the previous section, namely,

$$f(t) = e^{-t} - 2c^{-2t} + 3e^{-3t}. \tag{4}$$

Applying the above conditions, we get:

- $f(0) = 2 \geq 0$;
- $\lambda_3 f(0) + f'(0) = 6 - 6 = 0 \geq 0$; and
- $\lambda_3\lambda_2 f(0) + (\lambda_3 + \lambda_2) f'(0) + f''(0) = 12 - 30 + 20 = 2 \geq 0$.

Thus the second, and simpler test also works for this case.

However, neither of these tests is necessary as well as sufficient. To show this, consider the GH density offered as a Coxian example in O'Cinneide (1989), page 257, namely,

$$f(t) = 2(e^{-t}) - 3(2e^{-2t}) + 2(3e^{-3t}). \tag{5}$$

To check against the first set of conditions, we note that the numerator polynomial would have roots $(-1 \pm \sqrt{2}i)$, and thus $Re(\eta_1) = +1$. The scale parameters are $\theta_1 = 1, \theta_2 = 2, \theta_2 = 3$. Hence,

$$\frac{\theta_1 + \theta_2}{2} = \frac{3}{2} > Re(\eta_1) = 1,$$

and the condition is violated.

For the other set of conditions, we see that the second requirement is also violated, since

$$\lambda_3 f(0) + f'(0) = 6 - 8 < 0.$$

Furthermore, for a density as simple as

$$f(t) = 3(e^{-t}) - 3(2e^{-2t}) + (3e^{-3t}),$$

the first set of criteria is not even applicable since the numerator polynomial is the constant 1; all three of the requirements for the second set are, however, passed.

Next, we offer (as Lemma 2) another easily computed sufficient condition for determining whether a linear combination of exponentials (assumed to integrate to 1) is indeed a legitimate density function. For this, we need to partition the purported density $f(t)$ into two other functions depending on the sign of the specific a_i: $p(t)$ for those which are positive and $q(t)$ for those which are negative, such that $f(t) = p(t) - q(t)$, where both new functions are completely monotone sums of exponentials with positive multipliers. Then we have the following result.

Lemma 2: *The generalized hyperexponential function $f(t)$ will be a density if $ln\,(\bar{\lambda}q(0)/a_1\lambda_1)/(\lambda_2 - \lambda_1) < 0$ where $\bar{\lambda} = min\{\lambda_j : a_j > 0\}$.*

Proof: It is clear that, for very large t, $f(t)$ approaches $a_1\lambda_1 e^{-\lambda_1 t}$. Furthermore, we can observe that $p(t) \geq a_1\lambda_1 e^{-\lambda_1 t}$ and $q(t) \leq q(0)\bar{\lambda}e^{-\bar{\lambda}t}$. So if we can find a value t such that $a_1\lambda_1 e^{-\lambda_1 t} = q(0)\bar{\lambda}e^{-\bar{\lambda}t}$, then $p(t) \geq q(t)$ for all t greater than that value (call it s). It is easy to show that

$$s = \frac{ln\,(\bar{\lambda}q(0)/a_1\lambda_1)}{\lambda_2 - \lambda_1}. \tag{6}$$

The lemma then follows when $s < 0$. (Note the useful observation that the function $f(t)$ cannot have a root, that is, cannot intersect the t-axis, for any value larger than s even when $s > 0$.) □□

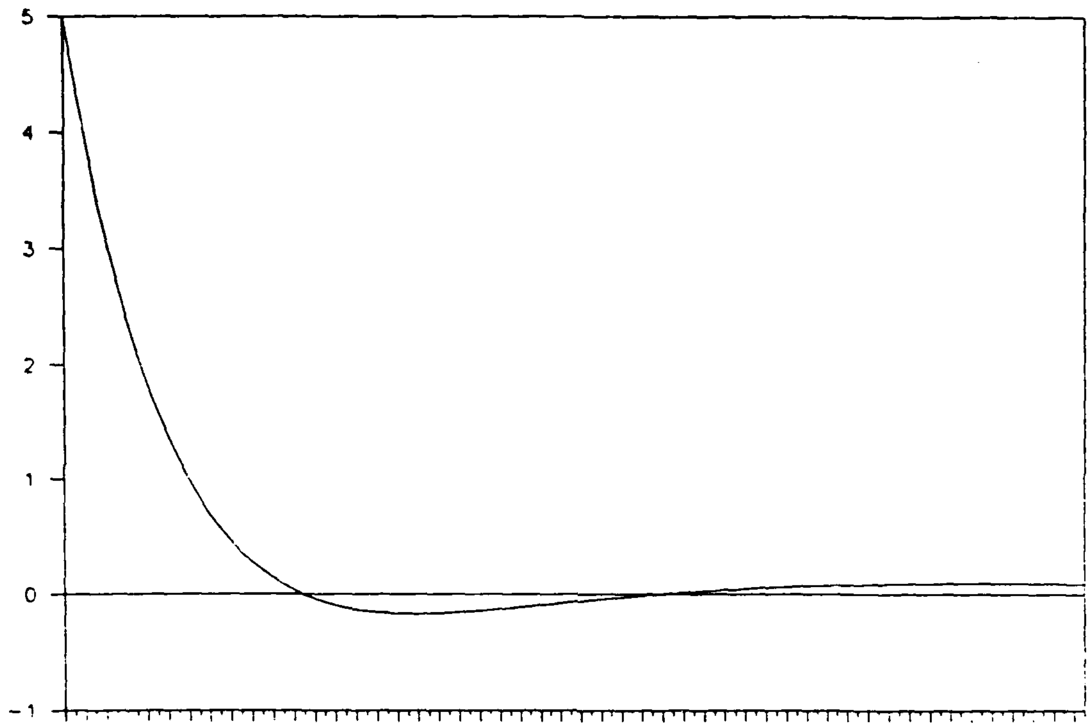
Even with this result, we need better ways to test. As we have seen, proper CDFs can fail to be picked up. No set of necessary and sufficient conditions has been found to validate, for example, such borderline possibilities as the function

$$f(t) = 2(e^{-t}) - 6(2e^{-2t}) + 5(3e^{-3t}).$$

At first glance, this linear combination would seem to be a satisfactory PDF. However, as can be seen in its plot in Figure 1, the function does indeed dip below the horizontal axis and is thus not legitimate. This experience suggests that plots can be very useful ways in performing the kind of analysis necessary. More on this in the next section.

Figure 1. Density Plot, I

$f(t) = 2(e^{-t}) - 6(2e^{-2t)} + 5(3e^{-3t})$



3 COMPUTATIONAL NECESSARY AND SUFFICIENT CONDITIONS

In this section, we offer some further thoughts on determining whether a linear combination of negative exponential functions is a proper density function. This will be done here through combined graphical and numerical means.

First, we repeat the old adage that "a picture is worth a thousand words." As we have noted with Figure 1, it is often quite easy to pick up density violations with carefully arrayed plots.

A more formal approach can be established by going back to our earlier decomposition of the potential generalized hyperexponential density $f(t) = p(t) - q(t)$. We provide a variation of Newton's method to find a root of $f(t)$ if it exists (i.e., to determine whether or not $f(t)$ ever violates the requirement that a PDF stay nonnegative). We do this by constructing a series of line segments which are both less than $p(t)$ and greater than $q(t)$ and eventually, together, move to the potential intersection of $p(t)$ with $q(t)$, that is, to a root of $f(t)$.

We begin from the calculation of the upper bound s of Lemma 2, beyond which there can be no roots to $f(t) = 0$. We start our Newton-like steps at the origin and move to s, with the procedure intended to locate any root which may exist along the way. If no root is found by s, then we would claim that the function is indeed a satisfactory PDF.

Specifically, a segment tangent to $p(t)$ with slope $p'(t)$ will always be less than $p(t)$, while a segment through the points t and s on the function $q(t)$ will be above the $q(t)$ over the range of interest. (See Figure 2.)

For any particular t, the two lines so constructed will have the following representations:

$$\begin{cases} y(x) = p'(t)(x-t) + p(t) \\ y(x) = m(x-t) + q(t) \end{cases}, \tag{7}$$

where $m = [q(s) - q(t)]/(s - t)$. Solution for the point of intersection leads to the recursive equation

$$t_{n+1} = t_n + \frac{p(t_n) - q(t_n)}{m_n - p'(t_n)}, \tag{8}$$

where $m_n = [q(s) - q(t_n)]/(s - t_n)$. Though this iteration is close to that of Newton's method, the step sizes here are actually somewhat smaller and we have a guarantee that no root is passed over at any step, with the iterants always staying to the left of the root. We quit when a t_n exceeds s.

By way of illustration, let us consider three examples, namely, those given earlier in Equations (2), (4) and (5). For the first case, we find that the upper bound is $s = ln\,(2/5) < 0$, and thus the function can have no roots over the positive real line and must be a density.

The second case has $s = ln\,3 = 1.099$, and the iterations follow as:

$$\begin{cases} t_0 &= 0 \\ t_1 &= 0.239 \\ t_2 &= 0.492 \\ t_3 &= 0.797 \\ t_4 &= 1.276 \end{cases} .$$

Thus this function is (once again) shown to be a legitimate density.

The third case has iterations (again with $s = 1.099$)

$$\begin{cases} t_0 &= 0 \\ t_1 &= 0.132 \\ t_2 &= 0.253 \\ t_3 &= 0.368 \\ t_4 &= 0.483 \\ t_5 &= 0.610 \\ t_6 &= 0.772 \\ t_7 &= 1.058 \\ t_8 &= 4.858 \end{cases} .$$

We have therefore been able to verify that (5) is a true density, something which we were *unable* to do with the conditions of the prior section.

However, our procedure will fail if the purported density is tangent (or very close to being so) to the time axis at a point less than the value of the computed upper bound s. Then the iterations will simply converge to the point of tangency and not go beyond.

So if the scanning procedure we have proposed should terminate before the value s is reached, we are not yet sure whether the function is a PDF. To deal with this we could then initiate a second scan from the right or positive side of the function, and a procedure analogous to the first scan can be applied.

Consider the point s. Construct a line tangent to $p(t)$ with slope $p'(t)$ through s. This line will be below the function $p(t)$. Construct a second line through the points $q(t_1)$ and $q(s)$, where t_1 is the value at which the first scan from the left appeared to terminate. This line will be above the function $q(t)$ in the range of interest.

Since $p(s) > q(s)$, the first line is above the second one at s and over some range to the left of s. Find the point of intersection. If it is to the right of s, then the first line is above the second throughout the range of interest and $p(t) > q(t)$. If the intersection point is to the left of s, then we know that $f(t)$ has no root between the intersection point and s. So we can successively scan from the right.

If the scanning from the right terminates at a value t_2 significantly different from t_1, then the function $f(t)$ must not be a PDF. This could be confirmed by computing $f'(t_1)$ and $f'(t_2)$. If $f'(t_1) < 0$ or $f'(t_2) > 0$, then $f(t)$ is not a PDF. On the other hand, if t_1 and t_2 are reasonably close, $f(t)$ may simply touch the axis at that point and still be a PDF. This could be confirmed by computing $f''(t_1) = f''(t_2)$. If $f''(t_1) = f''(t_2) > 0$, then $f(t)$ simply touches the axis without going below it.

In the scan from the right, the two equations [written in a form like that of Equation (7)] are:

$$\left\{ \begin{array}{rcl} y(x) & = & p'(s)(x - s) + p(s) \\ \\ y(x) & = & m_1(x - s) + q(s) \end{array} \right. ,$$

where $m_1 = [q(s) - q(t_1)]/(s - t_1)$. Solution for the point of intersection leads to the recursive equation:

$$s_{n+1} = s_n + [p(s_n) - q(s_n)]/[m_n - p'(s_n)],$$

where $m_n = [q(s_n) - q(t_1)]/(s_n - t_1), s_0 = s$.

Figure 2. Iterative Scheme Illustrating Convergence

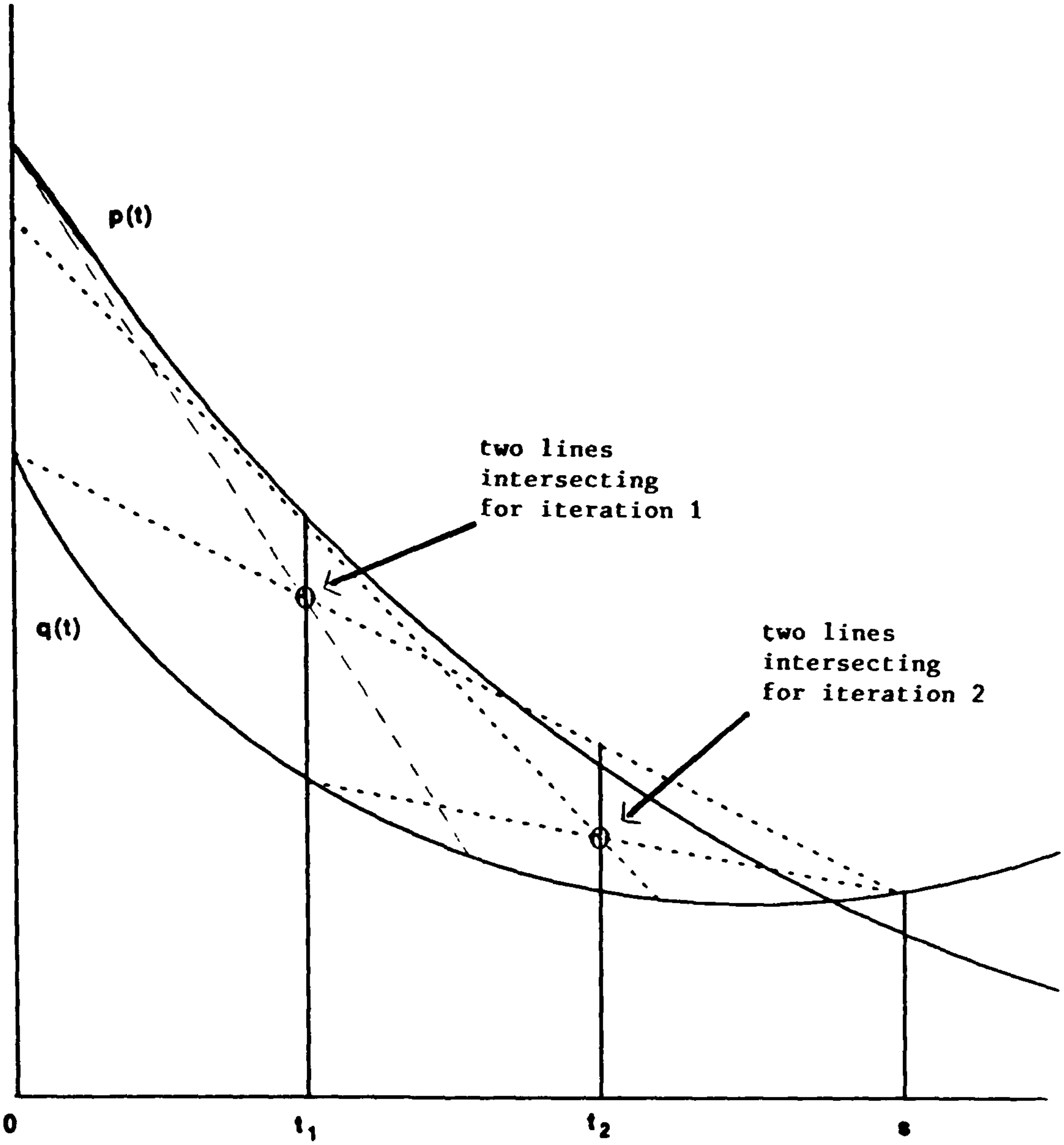
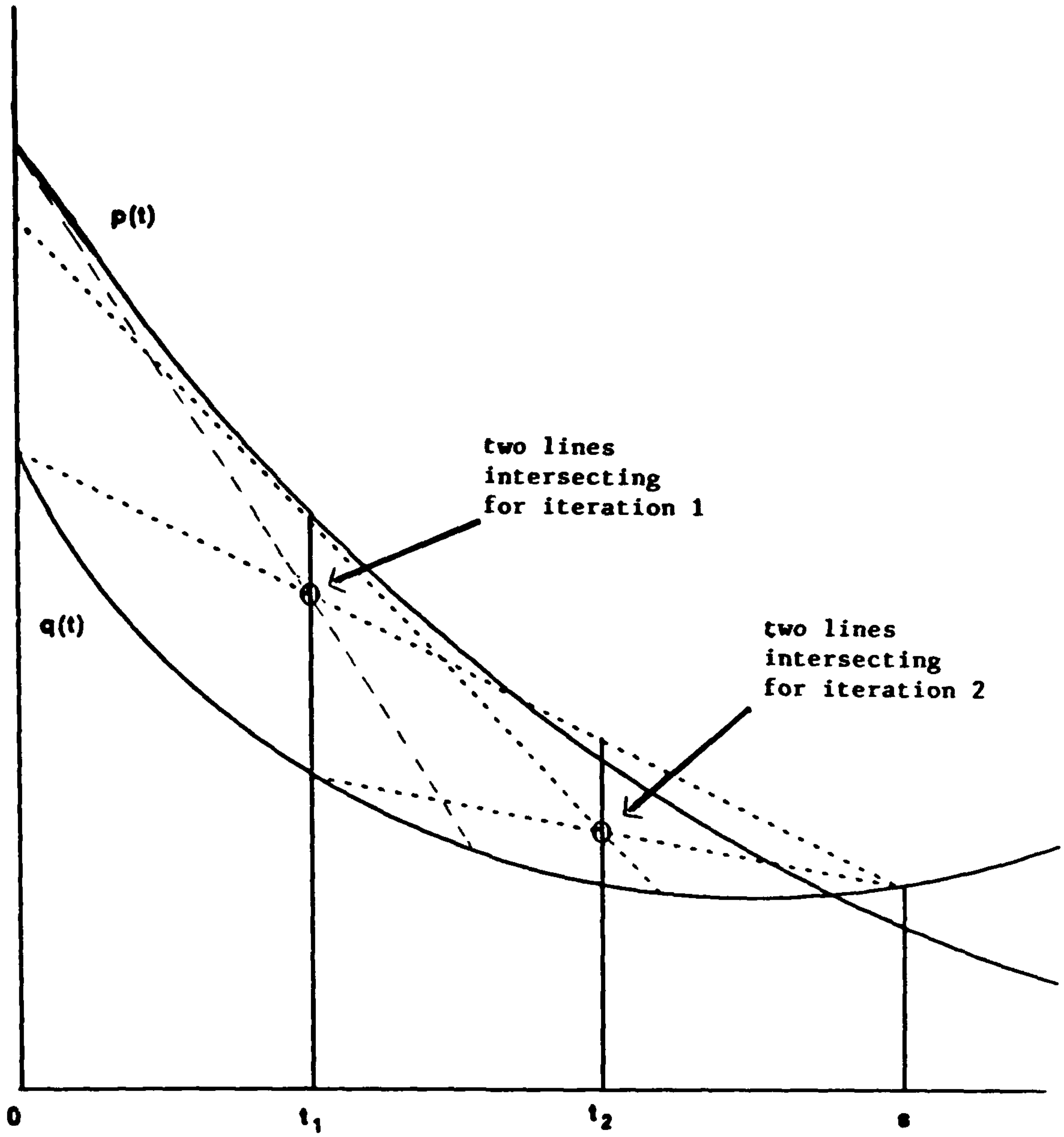


Figure 2. Iterative Scheme Illustrating Convergence



4 CONCLUDING REMARKS

We are now able to determine more completely whether given functions are true GH densities. Though our approach is partly numerical and thus not fully analytic, its implementation is very simple, and we have performed the necessary calculations on both '286- and '386-based desktop computers. In a sense then, this paper combines the latest in computational and graphic techniques with a theory which has evolved over many years beginning from the original work of Erlang.

Acknowledgments

This work was partially supported by ONR grant no. N00014-86-K-0029.

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